

# Spin Exciton Formation inside the Hidden Order Phase of CeB<sub>6</sub>

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The heavy fermion metal CeB<sub>6</sub> exhibits hidden order of antiferroquadrupolar (AFQ) type below  $T_Q = 3.2$  K and subsequent antiferromagnetic (AFM) order at  $T_N = 2.3$  K. It was interpreted as ordering of the quadrupole and dipole moments of a  $\Gamma_8$  quartet of localised Ce 4f<sup>1</sup> electrons. This established picture has been profoundly shaken by recent inelastic neutron scattering[1] that found the evolution of a feedback spin exciton resonance within the hidden order phase at the AFQ wave vector which is stabilized by the AFM order. We develop an alternative theory based on a fourfold degenerate Anderson lattice model, including both order parameters as particle-hole condensates of itinerant heavy quasiparticles. This explains in a natural way the appearance of the spin exciton resonance and the momentum dependence of its spectral weight, in particular around the AFQ vector and its rapid disappearance in the disordered phase. Analogies to the feedback effect in unconventional heavy fermion superconductors are pointed out.

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In strongly correlated f-electron metals the investigation of hidden order (HO) of unconventional non-magnetic type is a topic of central importance[2]. The most prominent and most investigated heavy fermion compounds that exhibit HO at low temperatures are URu<sub>2</sub>Si<sub>2</sub> and CeB<sub>6</sub> which have tetragonal ( $D_{4h}$ ) or cubic ( $O_h$ ) structure respectively. Two issues arise in the context of hidden order: Firstly, which symmetry is broken in the HO phase and to which irreducible representation the order parameter belongs. Secondly, should the ordering be described as appearance of spontaneous long range correlation between local f-electron degrees of freedoms, i.e. f-electron multipoles, or should HO rather be described as condensation of itinerant heavy particle-hole pairs with a nontrivial orbital structure. These opposite perspectives have prevented a clear identification of the HO in URu<sub>2</sub>Si<sub>2</sub> until present.

On the other hand since the work of Ohkawa[3] the HO in CeB<sub>6</sub> which appears at  $T_Q=3.2$  K has always been taken granted as a paradigm of the localised HO picture. In subsequent work along this line[4, 5] it was clarified that the primary HO parameter is of the two-sublattice antiferroquadrupolar (AFQ)  $\Gamma_5^+$  type ( $O_{yz}, O_{zx}, O_{xy}$ ) with wave vector  $\mathbf{Q}' = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$  in r.l.u.(R-point) which is nearly degenerate with an antiferrooctupolar (AFO)  $\Gamma_2^-$  ( $T_{xyz}$ ) order parameter which is strongly induced in an external field. Here  $\pm$  denotes the parity with respect to time reversal. The hidden multipolar order parameters are supported by the fourfold degenerate 4f crystalline electric field (CEF) ground state  $\Gamma_8$ . This localized scenario explains a large body of experimental results, including the field dependent increase and anisotropy of the critical temperature and the field induced Bragg peaks[6] at  $\mathbf{Q}'$  and NMR line shifts[5] although there is no macroscopic symmetry breaking observed [7]. A further important support for this picture comes from the predicted rapid field induced increase of the secondary octupole or-

der parameter[4] which was directly confirmed by RXS experiments[8]. At temperatures below  $T_N=2.3$  K finally CeB<sub>6</sub> develops antiferromagnetism (AFM) with  $\mathbf{Q} = (\frac{1}{4}, \frac{1}{4}, 0)$  ( $\Sigma$  or S -point) that coexists with AFQ order. Important information on HO may also be gained from the magnetic excitation spectrum. For finite fields that stabilizes the AFQ/AFO HO it was investigated within generalized Holstein-Primakoff and random phase approximation (RPA) approaches[9, 10]. Both lead to multipolar excitation bands in the range 1 – 2.5 meV and for finite applied field[11] their salient features agree with experimental results from inelastic neutron scattering (INS). In the numerous theoretical investigations of HO in CeB<sub>6</sub> the localised 4f approach was chosen and itinerant 4f character was completely neglected. This seems surprising because CeB<sub>6</sub> is a prominent example of a heavy fermion metal with one of the heaviest masses reported ( $m^*/m \geq 17$ )[12] and the Ce-dilute La-substitutes[13] being the standard case of Kondo resonance dominated local Fermi liquids with all the typical Kondo anomalies identified there. In fact the estimated Kondo temperature of the concentrated CeB<sub>6</sub> from quasielastic neutron scattering[14] is  $T^* \simeq 4.5$  K which is of the same order as  $T_Q$  and  $T_N$ . Therefore one question is whether the HO physics of CeB<sub>6</sub> can be completely explained within the conventional localized 4f approach.

Recent zero field high resolution INS experiments by Friemel et al[1] have indeed seriously questioned the standard picture and found intriguing new evidence that the dynamical magnetic response in the HO phase cannot be understood in the localized approach and, as in URu<sub>2</sub>Si<sub>2</sub>, requires taking into account the itinerant quasiparticle nature of f electrons. It was found that the low temperature magnetic response within the HO phase is determined by a pronounced *feedback effect*, i.e. a modification of magnetic spectral properties due to the appearance of order parameters: i) Below  $T_N$  a spin gap opens for low energies and spectral weight from the quasielastic

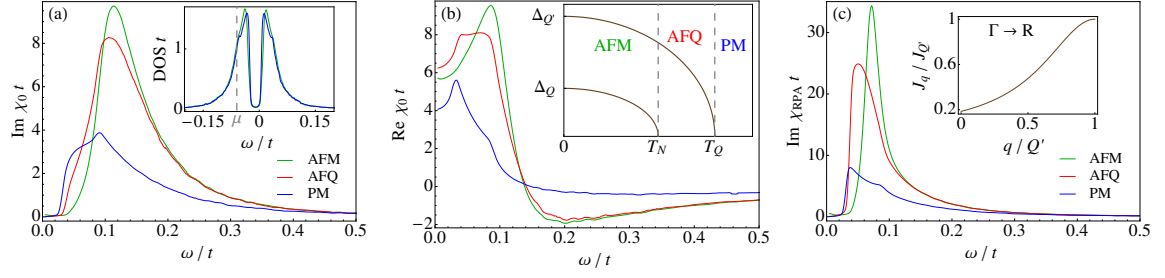


FIG. 1. (Color online) Non-interacting susceptibility at the R-point ( $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ ): (a) imaginary part and (b) real part. Inset of (a) shows the quasiparticle DOS in PM and coexisting AFQ/AFM ( $T=6 \times 10^{-3}t$ ) phase where  $\mu = -0.06t$  is the chemical potential. Inset of (b) gives the schematic temperature dependence of order parameters. quasiparticle model parameters:  $t = 22.4$  meV;  $\tilde{V} = 0.3t$ ;  $\tilde{\epsilon}_f = -0.01t$ ; gap parameters:  $\Delta_{Q'} = 0.015t$ ;  $\Delta_Q = 0.005t$  (c) Imaginary part of RPA susceptibility at R-point (inset shows the model for the quasiparticle interaction  $J_q$  along  $\Gamma R$  direction with  $J_{Q'} = 0.1t$ ).

region [15] is shifted to higher energies forming a pronounced resonance at  $Q'$  with peak position  $\omega_r \simeq 0.5$  meV. ii) Using the single-particle charge gap  $2\Delta \simeq 1.2$  meV in the HO phase from point-charge spectroscopy[16]  $\omega_r/2\Delta = 0.42 < 1$  is fulfilled showing that the resonance is indeed split off from the continuum. iii) The resonance appears mainly at the AFQ  $Q'$  but not at the AFM  $Q$  vector and shows no dispersion. Its intensity decreases rapidly when approaching  $T_N$  from below in an order-parameter like fashion. These characteristics of the magnetic spectrum in CeB<sub>6</sub> do not suggest a spin wave origin but rather are reminiscent of spin exciton resonances observed before in Fe-pnictide[17] and heavy fermion superconductors[18, 19] as well as Kondo insulators[20, 21]. The results of Ref.1 are the first clearcut example of the feedback spin exciton appearing within the AFQ HO phase. This proves that the localized 4f-scenario for CeB<sub>6</sub> is not adequate to explain its intriguing low energy spin dynamics and its momentum dependence.

In this Letter we therefore propose and explore an alternative route of theoretical modeling. We start from the central idea that the AFQ and AFM order parameters are to be described as particle hole condensates in the itinerant heavy quasiparticle picture. The latter is obtained from a microscopic fourfold ( $\Gamma_8$ -type) degenerate Anderson lattice model. It includes both twofold pseudo-spin ( $\sigma = \uparrow, \downarrow$ ) and twofold pseudo-orbital ( $\tau = \pm$ ) degeneracies of the hybridizing conduction (c) and 4f electron (f) in the  $\Gamma_8$  CEF ground state according to

$$\mathcal{H} = \sum_{\mathbf{k}, m} \left[ \epsilon_{\mathbf{k}}^c c_{\mathbf{k}m}^\dagger c_{\mathbf{k}m} + \epsilon_{\mathbf{k}}^f f_{\mathbf{k}m}^\dagger f_{\mathbf{k}m} + V_{\mathbf{k}} \left( c_{\mathbf{k},m}^\dagger f_{\mathbf{k}m} + h.c. \right) \right] + \sum_{i,m,n} U_{ff} f_{im}^\dagger f_{in} f_{in}^\dagger f_{im}. \quad (1)$$

where  $m = (\tau, \sigma)$  represents the fourfold  $\Gamma_8$  degeneracy. Here  $c_{\mathbf{k}m}^\dagger$  creates an conduction electron in the channel with corresponding  $\Gamma_8$  symmetry and wave vector  $\mathbf{k}$ . Furthermore,  $\epsilon_{\mathbf{k}}^c$  and  $\epsilon_{\mathbf{k}}^f = \epsilon^f$  are effective tight binding dispersions of the conduction band and the atomic

$f$  level position respectively. For the former we restrict to the next neighbor hopping ( $t$ ), i.e.,  $\epsilon_{\mathbf{k}}^c = 2t \sum_n \cos k_n$  ( $n = x, y, z$ ) which leads naturally to the AFQ ordering vector  $Q'$ . Furthermore  $f_{\mathbf{k}m}^\dagger$  creates the  $f$  electron with momentum  $\mathbf{k}$ , and  $U_{ff}$  is its on-site Coulomb repulsion. Finally  $V_{\mathbf{k}}$  is the hybridization energy between the lowest 4f doublet and conduction bands which contains in principle the effect of spin orbit and CEF but is taken as constant  $V_{\mathbf{k}} = V$  here.

In the limit  $U_{ff} \rightarrow \infty$  double occupation of the  $f$ -states are excluded, this is achieved by using the auxiliary boson  $b_i$  at each site  $i$ , with the constraint  $b_i^\dagger b_i + \sum_m f_{im}^\dagger f_{im} = 1$ . In the mean field (MF) approximation ( $r = \langle b_i \rangle = \langle b_i^\dagger \rangle$ ) diagonalization leads to hybridized quasiparticle bands[13]. They are determined by renormalized  $f$  level  $\tilde{\epsilon}_{\mathbf{k}}^f = \epsilon_{\mathbf{k}}^f + \lambda$  and effective (reduced) hybridization  $\tilde{V}_{\mathbf{k}} = rV_{\mathbf{k}}$ . Minimizing the MF ground state energy leads to selfconsistent equations for  $r, \lambda$ .

The AFQ and AFM order parameters with wave vectors  $Q$  and  $Q'$  respectively contribute extra MF terms

$$\begin{aligned} \mathcal{H}_{AFQ} &= \sum_{\mathbf{k}\sigma} \Delta_{Q'} (f_{\mathbf{k}+\sigma}^\dagger f_{\mathbf{k}+Q'-\sigma} + f_{\mathbf{k}-\sigma}^\dagger f_{\mathbf{k}+Q'+\sigma}), \\ \mathcal{H}_{AFM} &= \sum_{\mathbf{k}\tau} \Delta_Q (f_{\mathbf{k}\tau\uparrow}^\dagger f_{\mathbf{k}+Q\tau\downarrow} + f_{\mathbf{k}\tau\downarrow}^\dagger f_{\mathbf{k}+Q\tau\uparrow}). \end{aligned} \quad (2)$$

Our emphasis in this work is on the feedback effect, i.e. the effect of the gap opening within the HO phase on the magnetic response. Therefore we do not attempt a microscopic calculation to derive these order parameters and their temperature dependence. We include them as symmetry breaking molecular field terms in the Hamiltonian and take a generic empirical temperature dependence. The MF Hamiltonian  $\mathcal{H}_{MF}$  obtained from Eq. (1) is diagonalized by the unitary transformation

$$\begin{aligned} f_{\mathbf{k}m} &= u_{+, \mathbf{k}} a_{+, \mathbf{k}m} + u_{-, \mathbf{k}} a_{-, \mathbf{k}m} \\ c_{\mathbf{k}m} &= u_{-, \mathbf{k}} a_{+, \mathbf{k}m} - u_{+, \mathbf{k}} a_{-, \mathbf{k}m}. \end{aligned} \quad (3)$$

where  $2u_{\pm, \mathbf{k}}^2 = 1 \pm (\epsilon_{\mathbf{k}}^c - \tilde{\epsilon}_{\mathbf{k}}^f) / \sqrt{(\epsilon_{\mathbf{k}}^c - \tilde{\epsilon}_{\mathbf{k}}^f)^2 + 4\tilde{V}_{\mathbf{k}}^2}$ , lead-

ing to  $\mathcal{H}_{MF} = \sum_{i,\mathbf{k},m} E_{\mathbf{k}}^{\alpha} a_{\alpha,\mathbf{k}m}^{\dagger} a_{\alpha,\mathbf{k}m} + \lambda(r^2 - 1)$ , where

$E_{\mathbf{k}}^{\pm} = \frac{1}{2}[\epsilon_{\mathbf{k}}^c + \tilde{\epsilon}_{\mathbf{k}}^f \pm \sqrt{(\epsilon_{\mathbf{k}}^c - \tilde{\epsilon}_{\mathbf{k}}^f)^2 + 4\tilde{V}_{\mathbf{k}}^2}]$  are the pair ( $\alpha = \pm$ ) of hybridized quasiparticle ( $a_{\alpha\mathbf{k}m}$ ) bands, each fourfold ( $m=1-4$ ) degenerate. Here  $\tilde{V}_{\mathbf{k}}^2 = V_{\mathbf{k}}^2(1 - n_f)$  denotes the effective hybridization obtained by projecting out double occupancies. Due to  $1 - n_f \ll 1$   $\tilde{V}_{\mathbf{k}}$  is strongly reduced with respect to the single particle  $V_{\mathbf{k}}$  which leads to the large quasiparticle mass. Introducing new Nambu operators as  $\psi_{\mathbf{k}} = (C_{\mathbf{k}}, C_{\mathbf{k}+\mathbf{Q}}, C_{\mathbf{k}+\mathbf{Q}}^{\dagger})$  where  $C_{\mathbf{k}} = (b_{+, \mathbf{k}}, b_{-, \mathbf{k}})$  and  $b_{\alpha, \mathbf{k}}^{\dagger} = (a_{\alpha, \mathbf{k}+\uparrow}^{\dagger}, a_{\alpha, \mathbf{k}+\downarrow}^{\dagger}, a_{\alpha, \mathbf{k}-\uparrow}^{\dagger}, a_{\alpha, \mathbf{k}-\downarrow}^{\dagger})$ , we can write the total Hamiltonian  $\mathcal{H}_{tot} = \mathcal{H}_{MF} + \mathcal{H}_{AFQ} + \mathcal{H}_{AFM}$  as

$$\mathcal{H}_{tot} = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger} \hat{\beta}_{\mathbf{k}} \psi_{\mathbf{k}}; \quad \hat{\beta}_{\mathbf{k}} = \begin{bmatrix} \hat{E}_{\mathbf{k}} & \hat{\Delta}_{\mathbf{Q}'} & \hat{\Delta}_{\mathbf{Q}} \\ \hat{\Delta}_{\mathbf{Q}'}^{\dagger} & \hat{E}_{\mathbf{k}+\mathbf{Q}'} & 0 \\ \hat{\Delta}_{\mathbf{Q}}^{\dagger} & 0 & \hat{E}_{\mathbf{k}+\mathbf{Q}} \end{bmatrix},$$

here  $\hat{E}_{\mathbf{k}} = \hat{\mathcal{E}}_{\mathbf{k}} \otimes \tau_0 \otimes \sigma_0$ ,  $\hat{\Delta}_{\mathbf{Q}'} = \Delta_{\mathbf{Q}'}(\hat{\rho}_{\mathbf{k}, \mathbf{Q}'} \otimes \hat{\tau}_0 \otimes \hat{\sigma}_x)$ , and  $\hat{\Delta}_{\mathbf{Q}} = \Delta_{\mathbf{Q}}(\hat{\rho}_{\mathbf{k}, \mathbf{Q}} \otimes \hat{\tau}_x \otimes \hat{\sigma}_0)$ , where  $\hat{\mathcal{E}}_{\mathbf{k}}$  and  $\hat{\rho}_{\mathbf{k}, \mathbf{Q}'}$  are  $2 \times 2$  matrices in  $\alpha = \pm$  space with matrix elements  $\hat{\mathcal{E}}_{\mathbf{k}}^{\alpha\beta} = \delta_{\alpha\beta} E_{\mathbf{k}}^{\alpha}$ , and  $\hat{\rho}_{\mathbf{k}, \mathbf{Q}'}^{\alpha\beta} = u_{\alpha\mathbf{k}} u_{\beta, \mathbf{k}+\mathbf{Q}'}$ .  $\sigma_l, \tau_l$  are the Pauli matrices acting in pseudo-spin and pseudo-orbital space, respectively.

Defining the Matsubara Greens function (GF) matrix as  $\hat{G}_{\mathbf{k}}(\tau) = -\langle T \psi_{\mathbf{k}}(\tau) \psi_{\mathbf{k}}^{\dagger}(0) \rangle$ , and solving the standard equations of motion, one can find  $\hat{G}_{\mathbf{k}}(\omega_n) = (i\omega_n - \hat{\beta}_{\mathbf{k}})^{-1}$  which can be written as

$$\hat{G}_{\mathbf{k}}(\omega_n) = \begin{bmatrix} \hat{G}_{\mathbf{k}}^0 & \hat{G}_{\mathbf{k}, \mathbf{k}+\mathbf{Q}'}^0 & \hat{G}_{\mathbf{k}, \mathbf{k}+\mathbf{Q}}^0 \\ \hat{G}_{\mathbf{k}+\mathbf{Q}', \mathbf{k}}^0 & \hat{G}_{\mathbf{k}+\mathbf{Q}'}^0 & \hat{G}_{\mathbf{k}+\mathbf{Q}', \mathbf{k}+\mathbf{Q}}^0 \\ \hat{G}_{\mathbf{k}+\mathbf{Q}, \mathbf{k}}^0 & \hat{G}_{\mathbf{k}+\mathbf{Q}, \mathbf{k}+\mathbf{Q}'}^0 & \hat{G}_{\mathbf{k}+\mathbf{Q}}^0 \end{bmatrix}, \quad (4)$$

here  $\hat{G}_{\mathbf{k}}^0$  is a  $8 \times 8$  Green's function matrix in  $(\alpha, m)$  space. For the magnetic excitation spectrum we need the dipolar susceptibility matrix given by  $\chi_{\mathbf{q}}^{ll'}(t) = -\theta(t) \langle T j_{\mathbf{q}}^l(t) j_{-\mathbf{q}}^{l'}(0) \rangle$ , where  $j_{\mathbf{q}}^l = \sum_{\mathbf{k}m m'} f_{\mathbf{k}+\mathbf{q}m}^{\dagger} \hat{M}_{mm'}^l f_{\mathbf{k}m'}$  are the physical magnetic dipole operators ( $l, l' = x, y, z$ ). In cubic symmetry it is sufficient to calculate  $\chi_{\mathbf{q}}^{zz}(\omega)$ , corresponding to [10]  $\hat{M}^z = \frac{7}{6} \hat{\tau}_0 \otimes \hat{\sigma}_z$ , defining  $s = (\alpha, \mathbf{k} + \mathbf{q}, m_1)$  and  $s' = (\alpha', \mathbf{k}, m_2)$  one finds

$$\chi_0(\mathbf{q}, \omega) = \chi_{\mathbf{q}}^{zz}(\omega) \propto \sum_{\alpha\alpha' \mathbf{k} m_1 m_2} (\hat{\rho}_{\mathbf{k}, \mathbf{q}}^{\alpha'\alpha})^2 \int d\omega' \hat{G}_{ss'}^0(\nu + \omega') \hat{G}_{s's'}^0(\omega') |_{i\nu \rightarrow \omega + i0^+} \quad (5)$$

Here the  $\hat{\rho}_{\mathbf{k}, \mathbf{q}}^{\alpha'\alpha}$  are the matrix elements of reconstructed quasiparticle states in the AFQ/AFM state. They play a similar role as the 'coherence factors' in the spin excitation formation in unconventional superconductors. The dynamic magnetic susceptibility in RPA has the form

$$\chi_{RPA}(\mathbf{q}, \omega) = [1 - J_{\mathbf{q}} \chi_{\mathbf{q}}^{zz}(\omega)]^{-1} \chi_{\mathbf{q}}^{zz}(\omega), \quad (6)$$

where  $J_{\mathbf{q}}$  is the heavy quasiparticle interaction taken diagonal in  $(\alpha, m)$  band indices. In principle it is

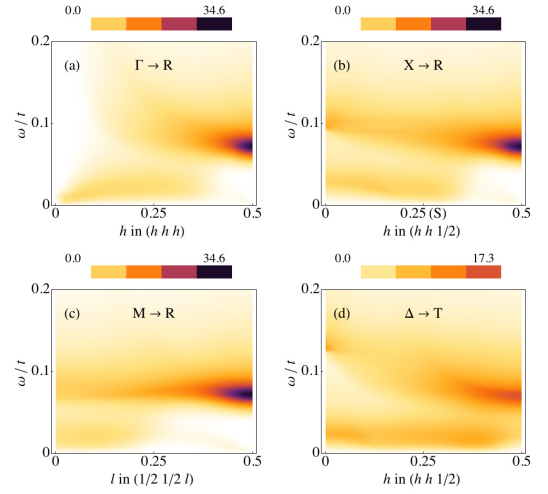


FIG. 2. (Color online) Contour plot of imaginary part of RPA dynamical susceptibility (a) from  $\Gamma(0\ 0\ 0)$  to  $R(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$ ; (b) from  $X(0\ 0\ \frac{1}{2})$  to  $R$ -point; (c) from  $X$ -point to  $R$ -point; (d) from  $\Delta(0\ 0\ \frac{1}{2})$  to  $T(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{4})$  (note different scale). Resonance is located around  $R$  and shows little dispersion.

determined by processes beyond the slave boson MF approximation[22]. However as in other spin-exciton theories[21, 23] we adopt here an empirical form of Lorentzian type that is peaked at the AFQ ordering vector where the resonance appears.

We will now discuss the characteristics of the magnetic excitation spectrum obtained from  $\chi_{RPA}''(\mathbf{q}, \omega)$  and show that it explains all the essential experimental features observed in  $\text{CeB}_6$ . In accordance with the heavy quasiparticle mass in this compound the chemical potential is chosen close to the top of the lower quasiparticle band (Fig. 1a inset:  $\mu = -0.06t$ ) where dispersion is flat, leading to a realistic mass enhancement  $m^*/m \simeq 20$ . All other model parameters are defined in Fig. 1.

First the spectrum  $\chi_0''(\mathbf{q}, \omega)$  of *non-interacting* quasiparticles is shown in Fig. 1a with constant- $\mathbf{q}$  scans for the paramagnetic (PM), AFQ and coexistent AFQ/AFM phases, respectively. In the PM state the spectrum exhibits the cf- hybridization gap at the  $R$ -point. When the AFQ, AFM order appears their corresponding gaps  $\Delta_{\mathbf{Q}'}$  and  $\Delta_{\mathbf{Q}}$  push the magnetic response to higher energies. The associated real part in Fig. 1b then shows a much enhanced response at these energies. As a consequence the magnetic spectrum for the *interacting* quasiparticles may develop a resonance when the real part of the denominator in Eq. (6) is driven to zero equivalent to a pole in  $\chi_{RPA}(\mathbf{Q}', \omega)$ . Due to the 3D electronic structure  $\chi_0'(\mathbf{Q}', \omega)$  will not be singular and the resonance will only appear for  $J(\mathbf{Q}')$  larger than a threshold value. The imaginary part is generally non-zero but small leading to a large resonant response at the pole position. The resonance appears in the HO phase when  $J_{\mathbf{Q}'} / t$  lies in a reasonable range such that the pole exists only when the

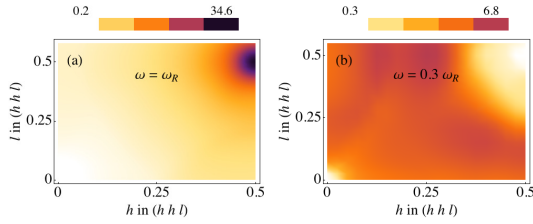


FIG. 3. (Color online) Contour plot of imaginary part of RPA dynamical susceptibility in (hhl)-plane of the reciprocal space; (a) at  $\omega = \omega_r = 0.07t$  (spin exciton resonance energy) pronounced localized peak at R-point appears (b) for energy in the spin gap, i.e.,  $\omega = 0.3\omega_r$ . Intensity at R-point vanishes due to spin gap formation.

real part is enhanced by the gap formation. Then the resonance condition  $1 = J_{\mathbf{Q}'}\chi_0(\mathbf{Q}', \omega_r)$  is fulfilled only in the AFQ ordered regime. The magnetic spectrum of interacting quasiparticles is shown in Fig. 1c. It shows indeed a peak appearing in the AFQ phase and a sharp resonant peak at  $\omega_r/2\Delta_c = 0.64$  at low temperature when both gaps are present. Here  $\Delta_c = 0.056t$  is the charge gap given in the inset of Fig. 1a. This explains the central observation of the R-point resonance in CeB<sub>6</sub>.

The momentum dependence of the spectrum in the AFQ/AFM phase and in particular the resonance peak is shown in Fig. 2 as contour plot in the  $\mathbf{q}, \omega$  plane with the wave vector  $\mathbf{q}$  chosen along various symmetry directions. There are two main characteristics: i) The single-particle spin gap due to the hybridization and enhanced by the AFQ/AFM gap formation appears most prominently close to the R point and less at other symmetry points like, e.g.,  $T(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$ . ii) The many-body resonance peak is also strongly constrained to the narrow region around the R-point, partly due to the suppression of the  $\chi'_0(\mathbf{q}, \omega)$  peak (Fig. 1b) when  $\mathbf{q}$  moves away from  $R(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$  and partly due to the decrease of  $J_{\mathbf{q}}$ . Both mean that the above condition for the resonance can only be fulfilled in a narrow region around the R-point where it is almost dispersionless. This corresponds exactly to the experimental observation in CeB<sub>6</sub> and similar observations have been made in the Ce-based superconductors [18, 19]. A complementary constant- $\omega$  plot of the magnetic scattering intensity which is proportional to  $\chi''_{RPA}(\mathbf{q}, \omega = \text{const})$  is shown in Fig. 3 for  $\mathbf{q}$  in the (hhl) plane as in the experimental scattering geometry. At the resonance position  $\omega_r$ , (a) the momentum dependent scattering intensity is strongly peaked at the R-point with rapid decay in all  $\mathbf{q}$  directions into the scattering plane. On the other hand for  $\omega = 0.3\omega_r$  (b) which is in the spin gap region, the latter shows up as a complete depletion of intensity at the R-point. Due to the magnetic sum rule the formation of the spin gap at this energy leads to a roughly even redistribution of the spectral weight across the whole scattering plane. This complete change of constant- $\omega$  intensity in (hhl) plane for  $\omega = \omega_r$  and

$\omega \ll \omega_r$  is in agreement with the experimental result[1].

Now we discuss the temperature dependence of resonance intensity. We start from itinerant type AFQ/AFM order parameters in Eq. (2) with a typical MF BCS temperature dependence shown in Fig. 1b (inset). The resonance intensity at the HO wave vector in Fig. 1c appears already at  $T_Q$  and is further enhanced below  $T_N$ . Experimentally it is found that it is strongly suppressed in the region  $T_N < T < T_Q$ . This is an effect of quadrupole OP fluctuations at zero field due to the near degeneracy with octupole order[24] which strongly suppress its amplitude. For example specific heat jump  $\Delta C(T_Q)$  for  $H=0$  is almost absent[25] while  $\Delta C(T_N)$  is pronounced. However in finite fields of a few Tesla the AFQ HO is stabilized and  $\Delta C(T_Q, H)$  is strongly enhanced. The stabilization of  $\Delta_{\mathbf{Q}'}$  in field is also directly known from RXS experiments[8]. This effect will also be present for the dynamical resonance. We therefore predict that the resonance peak at R will appear already in the temperature range  $T_N < T < T_Q$  when comparable fields are applied. We note that even in the case of a single superconducting order parameter the temperature dependence of the intensity generally deviates from the BCS MF behaviour.

In summary the recent INS experiments[1] require a rethinking of the HO phenomena in CeB<sub>6</sub>. The appearance of an itinerant spin exciton resonance at the AFQ wave vector  $\mathbf{Q}'$  proves that the previous restriction to localized 4f states in CeB<sub>6</sub> for the hidden AFQ order is oversimplified. The neglect of itinerant aspects can no longer be upheld. The theory presented here is therefore built on the delocalized heavy quasiparticle states. They are gapped due to the effect of hybridization and AFQ/AFM type particle-hole condensation leading to an enhanced magnetic response at the R-point. Due to quasiparticle interaction a pronounced spin exciton resonance at this wave vector appears. Its salient features of momentum, energy and temperature dependence are in agreement with experimental observation. Therefore CeB<sub>6</sub> is the first non-superconducting heavy fermion example with a spin exciton resonance excitation originating in the AFQ hidden order state.

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